Direct numerical simulations of electrophoresis of charged colloids : Smoothed profile method

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コロイド分散系における電気泳動現象では静電相互作用と流体力学相互作用のカップリングが本質的に重要である。本発表ではコロイド分散系の電気流体力学方程式を直接数値計算するシミュレーション手法である Smoothed Pro le(SP) 法を紹介する。いくつかのデモンストレーションを紹介し、電気泳動現象について古典的理論との比較などをおこないSP 法によるシミュレーションの有効性、妥当性を議論する。

Electrohydrodynamic phenomena are of great importance in physical, chemical, and biological science, and also in several engineering elds. In the case of electrophoresis of charged particles for example, the particles start to move on the application of external electric elds. The electric double layer, *i.e.* the cloud of counterions around charged particles, tends to be deformed and its distribution becomes anisotropic because of the applied external eld and also of the friction between ions and uids. In this situation, the time evolutions of the colloidal particles, the ions, and the host uids are described by coupled equations of hydrodynamics (Navier–Stokes) and electrostatics (Poisson) with proper boundary conditions imposed on the surfaces of the colloidal particles. However, the usual numerical techniques of partial di erential equations are hopeless to deal with dynamical evolutions of many-particle systems since the moving particle- uid boundary condition must be treated at every discrete time step.

Recently, we developed a reliable and efficient numerical method, called smoothed pro le (SP) method [1, 2], to resolve the hydrodynamic interactions acting on solid particles immersed in Newtonian host uids. In the SP method, the original sharp boundaries between colloids and host uids are replaced with di use interfaces with nite thickness ξ. This simple modi cation greatly improve the performance of numerical computations since it enables us to use the xed Cartesian grid even for the problems with moving boundary conditions.

The SP method is not only applicable to the dispersions in Newtonian uids, but particularly suitable for the particle dispersions in complex uids. It has already been applied successfully to liquid crystal colloidal dispersions [3, 4] and charged colloidal dispersions [5]. Field-particle

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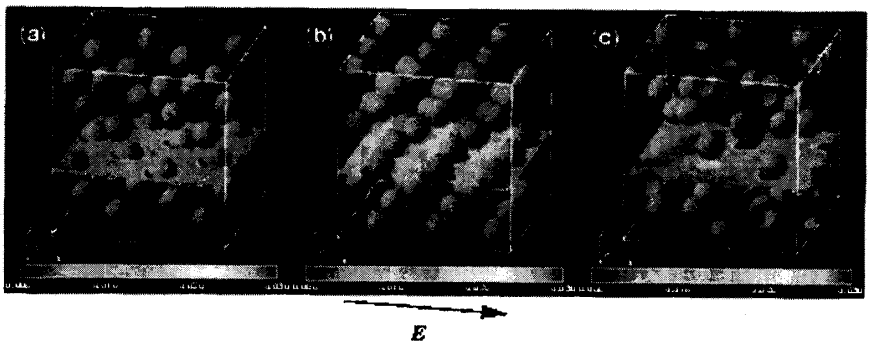

Figure 1: Snapshots of the electrophoresis of dense dispersions with (a) FCC, (b) BCC, and (c) random particle con gurations. The contour map represents the total ionic charge density in a plane perpendicular to z axis. The electric eld is applied in $+x$ direction normal to (1,0,0) face for FCC and BCC.

hybrid simulations were performed, where the average direction of the liquid crystal molecules and the density of ions were treated as coarse-grained continuum objects while colloids were treated explicitly as particles. The interaction between elds and particles were taken through the di use interface. The purpose of the present study is to establish an efficient and reliable simulation method applicable for electrohydrodymanic phenomena such as electrophoresis by combining our SP methods for hydrodynamic and electrostatic interactions [6].

In the presentation, we brie y outline our numerical modeling for charged colloidal dispersions and then demonstrate the reliability of the combined SP method by comparing our numerical results with classical approximation theories as to electrophoresis. Finally, comparisons are made for the electrophoretic mobilities of dense dispersions (Fig. 1), where the simulation results show notable deviations from a mean- eld type theory according to the cell model.

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